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On the mathematical model of triangulanes

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Abstract

The mathematical model of spirocondensed cyclopropanes, suggested by S.S. Tratch, is considered in the paper. According to the model every such compound is represented by a set of congruent equilateral triangles connected to each other by specific rules. One can associate an abstract graph with such a configuration of triangles. We investigate under what conditions a given graph can be realized as a graph of some spatial triangle configuration.

1. Introduction

A few years ago a new class of organic compounds was first investigated by N.S. Zefirov and his colleagues (see [10, 12]). This class (defined in [5, 10] as "triangulanes") consists of hydrocarbons whose skeleton is constructed only from triangles. Each triangle in every triangulane corresponds to a spiroattached three-membered ring.

At first sight, triangulanes seem to be very exotic and rare compounds. However, an intensive search arranged by discoverers of triangulanes made it possible to synthesize a considerable number of different compounds (see e.g. [6, 7, 11]). This success stimulated such theoretical investigations as enumeration of triangulanes, consideration of their stereoisomerism, construction of "synthetic trees" etc. All these investigations were based on the mathematical model of triangulanes suggested in [9, 10] by Tratch. This model initially treats triangulanes as a system of congruent equilateral triangles disposed in 3-dimensional space; such a system satisfies a few special requirements. Starting from this model and using his notion of an abstract configuration (see, for example [4, 8]) Tratch succeeded in ignoring metrical characteristics of molecular shapes of triangulanes. To every triangulane a certain characteristic graph was associated and all "essentially different" arrangements of such graphs in 3-dimensional space were

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enumerated for a special case when the graph is a chain, i.e., a tree in which all but two vertices have valency 2.

To date, among the triangulanes being synthesized, a few are known whose characteristic graph is a tree different from a chain (see [6, 7, 11]). However in all known cases such a graph has no cycles. This empirical fact has stimulated us to answer the following question: can there exist a triangulane whose characteristic graph is not a tree?

A negative answer on this question is presented in Section 3 on the assumption that instead of real chemical triangulanes their ideal mathematical model is considered. In Section 4 we consider Tratch's model of triangulanes more carefully and give a proof of certain of its properties which were not presented in [9, 10] in rigorous and evident form. We restrict ourselves to considerating chain triangulanes, which have a tree as a characteristic graph.

In Section 4.1 all congruence classes of chain triangulanes with n triangles are described in terms of a special $(n-4)$-dimensional coarse code. In the next subsection a finer $(n-3)$-dimensional τ-code makes it possible to distinguish classes of rotation-congruent triangulanes. Section 4.3 concerns the notion of non-regular triangulanes.

In the final Section 5 we discuss the relationship between our ideal mathematical model and real chemical triangulanes. The possibilty of the existence of real chemical cycle triangulanes is mentioned. Certain ways to arrange more flexible rules for the description of spatial model of chemical triangulanes are briefly discussed.

2. Preliminaries

We define an *ideal mathematical triangulane* (in what follows we shall consider only these ones and shall call them simply triangulanes) as a finite set of congruent equilateral triangles disposed in 3-dimensional Euclidean vector space. It is convenient for us to fix a length of triangle side equal to $\sqrt{\frac{3}{2}}$. The radius of a circle circumscribed about such a triangle is equal to $\sqrt{2}/2$.

We shall say that two triangles are *adjacent* if they satisfy the following conditions (see Fig.1):

(i) they have a common vertex which is their unique intersection point;

(ii) triangle planes are orthogonal;

(iii) the line which connects the triangle centres passes through their common vertex.

We shall say that n congruent regular triangles disposed in $\mathbf{R}^3$ form a *regular triangulane* if any two triangles are either adjacent or have an empty intersection (by triangle we mean a triangle together with an internal part of its plane). One can associate with any triangulane an abstract graph whose vertices are the triangles and where two vertices are connected by an edge if and only if the corresponding triangles are adjacent in the triangulane. A triangulane is said to be *connected* if and only if its graph is connected. Later on we shall consider only connected triangulanes.

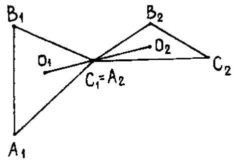

Fig. 1.

We shall say that two triangulanes are *congruent* if one can be transformed onto another by means of an Euclidean transformation. The following question is central to the paper. To describe, up to the congruence, all regular triangulanes formed by n triangles. The notion introduced above of a triangulane graph allows us to split the initial problem into two:

(i) To characterize all graphs of regular triangulanes;

(ii) For a given graph Γ to enumerate all non-congruent regular triangulanes having Γ as a graph.

Traingulanes having a chain as a graph (here and later we shall call them *chain triangulanes*) were considered in [9, 10], where they were called *unbranched triangulanes*. In [9, 10] a special kind of labelling of the sequences of chain vertices was suggested to distinguish non-congruent "oriented" triangulanes (see Section 4.2). The authors have also found a number of such labellings, but they have not considered in general when such a labelling may be realized, i.e. when there exists a regular chain triangulane corresponding to the given labelling.

It should be mentioned that the problem (i) was not considered in [9, 10] at all. Here we do the first step for its solution. We prove the following

Theorem 2.1. *Any ideal triangulane graph is a tree.*

The proof of the theorem is contained in Section 3.

3. An ideal triangulane graph has no cycle

This section contains the proof of Theorem 2.1. First we shall introduce some additional notions. We define *a sequence* of triangles as an ordered set $T_1, \dots, T_{n+1}$ of $n+1$ triangles such that T_i is adjacent with T_{i+1}. Let $r_1, \dots, r_{n+1}$ be centres of these triangles. Let $e_i = r_{i+1} - r_i$, $i = 1, \dots, n$.[2] Since length of triangle side is equal to $\sqrt{\frac{3}{2}}$ then $(e_i, e_i) = 2$ (we use a notation (,) for the standard scalar product in 3-dimensional Euclidean vector space $\mathbf{R}^3$). Due to the definition of adjacency relation one can easily see that the angle between two congruent vectors e_i and e_{i+1} is equal to $\pm\pi/3$ (see Fig. 2). Therefore, $(e_i, e_{i+1}) = 1$ for all $i = 1, \dots, n-1$.

Proposition 3.1. $(e_i, e_{i+2}) = \frac{1}{2}$.

[2] Here and later we shall identify points of $\mathbf{R}^3$ and their radius-vectors.

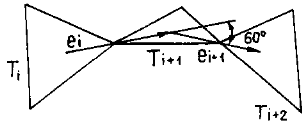

Fig. 2.

Proof. Let us consider four consecutive triangle centres $r_i, r_{i+1}, r_{i+2}, r_{i+3}$. From the definition of the adjacency relation we see that the ends of the vectors r_i, r_{i+1}, r_{i+2} lie in the plane of the triangle T_{i+1}. Analogously, ends of vectors $r_{i+1}, r_{i+2}, r_{i+3}$ lie in the plane of the triangle T_{i+2}. Since T_{i+1} and T_{i+2} are adjacent their planes are orthogonal, which, in its own turn, is equivalent to an orthogonality of the planes $< r_{i+1} - r_i = e_i, r_{i+2} - r_{i+1} = e_{i+1} >$ and $< r_{i+3} - r_{i+2} = e_{i+2}, r_{i+2} - r_{i+1} = e_{i+1} >$. The planes $< e_i, e_{i+1} >$, $< e_{i+1}, e_{i+2} >$ are orthogonal iff $(e_i \times e_{i+1}, e_{i+1} \times e_{i+2}) = 0$ (here $\times$ is a vector product in $\mathbf{R}^3$). By using the known formula $(a \times b, c \times d) = (a,c)(b,d) - (a,d)(b,c)$ we obtain $(e_i \times e_{i+1}, e_{i+1} \times e_{i+2}) = (e_i, e_{i+1})(e_{i+1}, e_{i+2}) - (e_i, e_{i+2})(e_{i+1}, e_{i+1}) = 1 - (e_i, e_{i+2}) \cdot 2 = 0$, whence it follows $(e_i, e_{i+2}) = \frac{1}{2}$. □

Corollary 3.2. *For any consecutive triple of vectors e_i, e_{i+1}, e_{i+2}, $i = 1, \ldots, n-2$ the following equations hold:*

(i) $(e_i, e_i) = (e_{i+1}, e_{i+1}) = (e_{i+2}, e_{i+2}) = 2$;

(ii) $(e_i, e_{i+1}) = (e_{i+1}, e_{i+2}) = 1$;

(iii) $(e_i, e_{i+2}) = \frac{1}{2}$.

Lemma 3.3. *Let $e_1, \ldots, e_n$ be a sequence of vectors satisfying the conditions* (i)–(iii). *Then $(e_1, e_n) = (2m+1)/2^{n-2}$ for an appropriate integer m.*

The **proof** will be carried by induction on n. First we shall verify our statement for values $n = 1, 2, 3$.

$$n = 1 \quad (e_1, e_1) = 2 = \frac{2 \cdot 0 + 1}{2^{-1}},$$

$$n = 2 \quad (e_1, e_2) = 1 = \frac{2 \cdot 0 + 1}{2^0},$$

$$n = 3 \quad (e_1, e_3) = \frac{1}{2} = \frac{2 \cdot 0 + 1}{2^1}.$$

Induction step. We may assume that $n \geqslant 4$. It follows from properties (i)–(iii) that the vectors $e_{n-3}, e_{n-2}, e_{n-1}$ are linearly independent (because the matrix of their scalar products is non-degenerate). Therefore $e_n = \lambda_1 e_{n-1} + \lambda_2 e_{n-2} + \lambda_3 e_{n-3}$. Equalities (i)–(iii) of the Corollary 3.2 give us a system of equations:

$$2 = (e_n, e_n) = 2\lambda_1^2 + 2\lambda_2^2 + 2\lambda_3^2 + 2\lambda_1\lambda_2 + 2\lambda_2\lambda_3 + \lambda_1\lambda_3,$$

$$1 = (e_n, e_{n-1}) = 2\lambda_1 + \lambda_2 + \frac{1}{2}\lambda_3,$$

$$1/2 = (e_n, e_{n-2}) = \lambda_1 + 2\lambda_2 + \lambda_3.$$

This system has two solutions only:

$$\lambda_1 = \frac{1}{2},\ \lambda_2 = \frac{1}{2},\ \lambda_3 = -1,$$
$$\lambda_1 = \frac{1}{2},\ \lambda_2 = -\frac{1}{2},\ \lambda_3 = 1.$$

Thus, we have $e_n = \frac{1}{2}e_{n-1} \pm (\frac{1}{2}e_{n-2} - e_{n-3})$. By the induction hypothesis $(e_1, e_i) = (2k_i + 1)/2^{i-2}$, for all $i \leqslant n-1$. So we have

$$\begin{aligned}(e_n, e_1) &= \tfrac{1}{2}(e_{n-1}, e_1) \pm (\tfrac{1}{2}(e_{n-2}, e_1) - (e_{n-3}, e_1))\\ &= \frac{1}{2}\frac{2k_{n-1}+1}{2^{n-3}} \pm \left(\frac{1}{2}\frac{2k_{n-2}+1}{2^{n-4}} - \frac{2k_{n-3}+1}{2^{n-5}}\right)\\ &= \frac{2k_{n-1} + 1 \pm (4k_{n-2} + 2 - 16k_{n-3} - 8)}{2^{n-2}}\\ &= \frac{2(k_{n-1} \pm (2k_{n-2} - 8k_{n-3} - 3)) + 1}{2^{n-2}} = \frac{2k_n + 1}{2^{n-2}}. \quad \square\end{aligned}$$

Proof of the Theorem 2.1. Let T be any triangulane. Suppose that its graph is not a tree, i.e., it contains a cycle. That means there exist n triangles $T_1, \ldots, T_n$ such that T_i is adjacent with T_{i+1} for $i = 1, \ldots, n-1$ and T_n is adjacent with T_1. As above, r_i is a centre of triangle T_i, $e_i = r_{i+1} - r_i$, $i = 1, \ldots, n-1$ and $e_n = r_1 - r_n$. Since $T_1, \ldots, T_n, T_{n+1} = T_1$ is a sequence of triangles $(e_n, e_1) = (2k+1)/2^{n-2}$ for an appropriate integer k. On the other hand a triple T_n, T_1, T_2 is also a sequence of triangles, so, by the Corollary 3.2, $(e_n, e_1) = 1$. Thus, we have an equation $(2k+1)/2^{n-2} = 1$. One can easily verify that $k = 0$, $n = 2$ is the unique solution of the equation. But it is evident that two adjacent triangles cannot form a cycle. $\square$

The following question can be naturally raised now. What trees may occur as graphs of regular triangulanes? The evident restriction coming from the definition of the adjacency relation says that a valency of any tree vertex does not exceed 3. We shall not consider here more strong restriction and pay our attention to a case of chain triangulanes only.

4. Chain triangulanes

Recall that *a chain triangulane* is one whose graph is a chain. It is clear that any chain as an abstract graph is uniquely determined by the number of vertices. The main goal of this section is to describe all non-congruent chain triangulanes. As was mentioned above by the congruence here and later we mean a classical notion used in 3-dimensional Euclidean geometry. Two objects are *congruent* iff one of them can be superimposed onto the other by a sequence of the following transformations: translation, rotation, reflection. The last claim may be reformulated in the following manner: one can be moved onto the other by an Euclidian transformation L, where for $r \in \mathbf{R}^3$, $L(r) = P(r) + b, P$ is an orthogonal transformation of $\mathbf{R}^3$, and $b \in \mathbf{R}^3$. Chain triangulanes and congruence relation on them were considered for the first time in [9, 10]. Here we give a more rigorous treatment of this subject.

4.1. Congruence classes of chain triangulanes

In this subsection we construct a code which is complete invariant of congruence classes of chain triangulanes .

Proposition 4.1. *Any two chain triangulanes with the same number $n \leqslant 4$ of triangles are congruent.*

Proof. The statement can be easily verified for $n = 1,2,3$. $n = 4$ is the only case we need to prove. Let $\boldsymbol{T} = \{T_1, T_2, T_3, T_4\}$ and $\boldsymbol{S} = \{S_1, S_2, S_3, S_4\}$ be two chain triangulanes. Since our statement is valid for $n=3$ there exists an Euclidean transformation L which moves S_i onto T_i, $i = 1,2,3$. Triangulanes $\boldsymbol{S} = \{S_1, S_2, S_3, S_4\}$ and $L(\boldsymbol{S}) = \{L(S_1), L(S_2), L(S_3), L(S_4)\} = \{T_1, T_2, T_3, L(S_4)\}$ are congruent, hence we may consider the last one instead of $\boldsymbol{S}$. If $L(S_4) = T_4$ then there is nothing to prove. If it is not the case, then 4-tuple $\{T_1, T_2, T_3, T_4\}$ can be transformed onto $\{T_1, T_2, T_3, L(S_4)\}$ by an orthogonal reflection of the plane of the triangle T_2 (see Fig.3). $\square$

Let $\boldsymbol{T} = \{T_1, \ldots, T_5\}$ be a chain triangulane and r_i be a centre of triangle T_i, $i = 1, \ldots, 5$. Consider vectors $e_i = r_{i+1} - r_i$, $i = 1, \ldots, 4$. It follows from the proof of Lemma 2.3 that $e_4 = \frac{1}{2}e_3 \pm (\frac{1}{2}e_2 - e_1)$. So we define *a sign* $s(T_1, \ldots, T_5)$ of the ordered 5-tuple $(T_1, \ldots, T_5)$ as $+1$ if $e_4 = \frac{1}{2}e_3 + (\frac{1}{2}e_2 - e_1)$ and -1 otherwise. The following proposition shows the connection between $s(T_1, \ldots, T_5)$ and $s(T_5, \ldots, T_1)$.

Proposition 4.2. $s(T_1, \ldots, T_5) = s(T_5, \ldots, T_1)$.

Proof. We consider the case $s(T_1, \ldots, T_5) = +1$ only, because the (-1)-case has an analogous proof. In this case $e_4 = \frac{1}{2}e_3 + \frac{1}{2}e_2 - e_1$, whence it follows $-e_1 = \frac{1}{2}(-e_2) + \frac{1}{2}(-e_3) - (-e_4)$. To complete the proof it is sufficient to write the following equality: $r_i - r_{i+1} = -e_i$, $i = 1, \ldots, 4$. $\square$

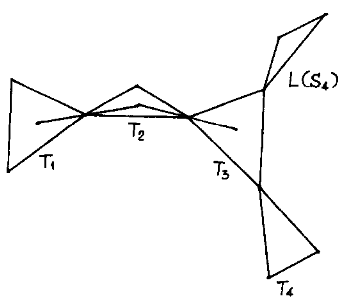

Fig. 3.

By using the sign function we can give an exact description of the congruence classes of the chain triangulanes.

Theorem 4.3. *Let* $\boldsymbol{T} = (T_0, \ldots, T_n)$ *and* $\boldsymbol{S} = (S_0, \ldots, S_n)$, $n \geqslant 4$ *be two chain triangulanes. They are congruent if and only if at least one of the following two conditions is satisfied:*

(i) $s(T_i, T_{i+1}, T_{i+2}, T_{i+3}, T_{i+4}) = s(S_i, S_{i+1}, S_{i+2}, S_{i+3}, S_{i+4})$ *for each* $i \leqslant n-4$;

(ii) $s(T_i, T_{i+1}, T_{i+2}, T_{i+3}, T_{i+4}) = s(S_{n-i}, S_{n-(i+1)}, S_{n-(i+2)}, S_{n-(i+3)}, S_{n-(i+4)})$ *for each* $i \leqslant n-4$.

Proof. Suppose at first that they are congruent, i.e., there exists an Euclidean transformation L which moves $\boldsymbol{T}$ onto $\boldsymbol{S}$. It is evident that $L(T_0)$ is either S_0 or S_n. Without loss of generality we can assume that $L(T_0) = S_0$. Since L preserves the adjacency relation, then $L(T_i) = S_i$, which implies $L(r_i) = q_i$, where r_i and q_i are the centres of T_i and S_i, respectively.

Let L have a form $L(r) = P(r) + b$, where P is an orthogonal transformation of $\mathbf{R}^3$ and b is an arbitrary vector. So we have $q_i = P(r_i) + b$. Let us denote for convenience $s(T_i, \ldots, T_{i+4})$ by s_1 and $s(S_i, \ldots, S_{i+4})$ by s_2. Due to the definition of the sign function we have:

$$r_{i+3} - r_{i+2} = \frac{1}{2}(r_{i+2} - r_{i+1}) + s_1 \left(\frac{1}{2}(r_{i+1} - r_i) - (r_i - r_{i-1}) \right).$$

By applying of P to the both sides of the equality we obtain:

$$q_{i+3} - q_{i+2} = \frac{1}{2}(q_{i+2} - q_{i+1}) + s_1 \left(\frac{1}{2}(q_{i+1} - q_i) - (q_i - q_{i-1}) \right).$$

On the other hand, the following holds:

$$q_{i+3} - q_{i+2} = \frac{1}{2}(q_{i+2} - q_{i+1}) + s_2 \left(\frac{1}{2}(q_{i+1} - q_i) - (q_i - q_{i-1}) \right).$$

Comparing these two equalities, we get:

$$(s_1 - s_2) \left(\frac{1}{2}(q_{i+1} - q_i) - (q_i - q_{i-1}) \right) = 0.$$

Since $\|q_{i+1} - q_i\| = \|q_i - q_{i-1}\| = 2$ then vector standing within brackets is non-zero. Therefore $s_1 = s_2$.

Let us prove the second part of the statement. Suppose one of (i)–(ii) is true. We may assume that condition (i) is satisfied.[3] By the Proposition 4.1 there exists an Euclidean transformation $L(x) = P(x) + b$ which moves T_i onto $S_i, 0 \leqslant i \leqslant 3$. We claim that $L(T_j) = S_j$ for all $0 \leqslant j \leqslant n$. We shall prove this by induction on j. We can suppose

[3] The case when the condition (ii) is satisfied is reduced to this one by the renumbering $i \to n-i$ of triangles $S_0, \ldots, S_n$.

that $j \geqslant 4$. In this situation it is sufficient to prove that $L(r_j) = q_j$. Let us denote for convenience $s(T_{j-4},\dots,T_j) = s(S_{j-4},\dots,S_j)$ by s. Let r_j, q_j be centers of triangles T_j, S_j, respectively. Under this notation we can write

$$r_j - r_{j-1} = \frac{1}{2}(r_{j-1} - r_{j-2}) + s\left(\frac{1}{2}(r_{j-2} - r_{j-3}) - (r_{j-3} - r_{j-4})\right),$$

$$q_j - q_{j-1} = \frac{1}{2}(q_{j-1} - q_{j-2}) + s\left(\frac{1}{2}(q_{j-2} - q_{j-3}) - (q_{j-3} - q_{j-4})\right).$$

By application of P to both sides of the first equality and using an induction hypothesis we get:

$$L(r_j) - q_{j-1} = \frac{1}{2}(q_{j-1} - q_{j-2}) + s\left(\frac{1}{2}(q_{j-2} - q_{j-3}) - (q_{j-3} - q_{j-4})\right).$$

By comparing of this equality with the previous one we obtain $L(r_j) = q_j$. $\square$

Now we shall define a coarse code of a *chain* triangulane. Let $\chi_i = s(T_i, T_{i+1}, T_{i+2}, T_{i+3}, T_{i+4})$, $i = \overline{1, n-4}$. Let $\chi = (\chi_1,\dots,\chi_{n-4})$, $\chi^t = (\chi_{n-4},\dots,\chi_1)$. It is clear that $(\chi^t)^t = \chi$. Then a *coarse code* of a triangulane is a set $\{\chi, \chi^t\}$. It follows from Theorem 4.3 that the coarse code characterises a triangulane up to the congruence.

4.2. *r-congruence of triangulanes*

In the previous section we described congruence classes of chain triangulanes for the classical definition of the congruence. However, in chemistry another notion of congruence is also used. That is a congruence of "oriented" objects. We shall give its definition in the group-theoretical way. We shall say that two geometrical objects are *r-congruent* if and only if there exists a transformation $x \to P(x) + b$, with a *rotation* P, moving one of them onto another. It is clear that any two r-congruent objects are also congruent in the classical sense.

Tratch was the first who proposed a "$\pm$"-code for description of r-congruence of the chain triangulanes. He used this code for the enumeration of all possible chain triangulanes; however, he did not consider the question: does his code really describe classes of r-congruence. The main purpose of this subsection is to give the rigorous mathematical foundation of his code. To do this we recall some facts and definitions from elementary geometry.

Unlike the analysis of 3D-configurations used in [9, 10] we build the code suggested by Tratch (briefly τ-code) by means of the classical geometrical operations in 3-dimensional vector space $\mathbf{R}^3$ such as a vector product $\times$ and scalar one $(\ ,\ )$. We shall also use a well known invariant of the 3-dimensional rotation group called *a mixed product* of a vector triple a, b, c. It is defined by the following formula

$$[a,b,c] = ((a \times b), c).$$

We shall say that a vector triple a, b, c is *positively (negatively) oriented* if $[a,b,c] > 0$ (resp. $[a,b,c] < 0$). The statement below contains all the mixed product properties we need. We give it without proof.

Proposition 4.4. (i) *Let a, b, c be a vector triple, then*

$$[a,b,c] = [c,a,b] = [b,c,a] = -[b,a,c] = -[a,c,b] = -[c,b,a];$$

(ii) *for any rotation P it holds:* $[a,b,c] = [P(a), P(b), P(c)]$;

(iii) *let P be an orthogonal operator. If for some noncomplanar triple of vectors a, b, c the triple $P(a), P(b), P(c)$ has the same orientation as a, b, c has, then P is a rotation.*

Let $\{T_1, T_2, T_3, T_4\}$ be a chain triangulane and r_i be a centre of the triangle T_i. We define a sign $g(T_1, T_2, T_3, T_4)$ as $+1$ if a triple $r_2 - r_1, r_3 - r_2, r_4 - r_3$ is positively oriented and -1 otherwise.

Proposition 4.5. $g(T_1, T_2, T_3, T_4) = g(T_4, T_3, T_2, T_1)$.

Proof. As above r_i is a centre of T_i and $e_i = r_{i+1} - r_i$. Then, by definition, $g(T_1, T_2, T_3, T_4)$ is a sign of $[e_1, e_2, e_3]$ while $g(T_4, T_3, T_2, T_1)$ is a sign of $[-e_3, -e_2, -e_1]$. But one can easily prove an identity $[e_1, e_2, e_3] = [-e_3, -e_2, -e_1]$. □

Proposition 4.6. *Let $\{T_1, T_2, T_3, T_4, T_5\}$ be a chain triangulane. Then $s(T_1, T_2, T_3, T_4, T_5) = -g(T_1, T_2, T_3, T_4)\, g(T_2, T_3, T_4, T_5)$*

Proof. Let us denote, for convenience, $s(T_1, T_2, T_3, T_4, T_5)$ by λ. As usual, r_i is a centre of a triangle T_i and $e_i = r_{i+1} - r_i, i = 1,2,3,4$. Then $e_4 = \frac{1}{2}e_3 + \lambda(\frac{1}{2}e_2 - e_1)$ and $g(T_2, T_3, T_4, T_5) = [e_2, e_3, e_4] = -\lambda[e_2, e_3, e_1] = -\lambda[e_1, e_2, e_3] = -\lambda \cdot g(T_1, T_2, T_3, T_4)$. □

Now we are ready to construct a τ-code of a chain triangulane. Let $\boldsymbol{T} = \{T_1, \ldots, T_n\}$ be a chain triangulane. *A τ-code* of $\boldsymbol{T}$ is an unordered pair of two $(n-3)$-dimensional vectors ε and δ whose coordinates ε_i, δ_i are defined by the formula

$$\varepsilon_i = g(T_i, T_{i+1}, T_{i+2}, T_{i+3}), \quad i = \overline{1, n-3},$$
$$\delta_i = g(T_{n-i+1}, T_{n-i}, T_{n-i-1}, T_{n-i-2}), \quad i = \overline{1, n-3}.$$

Proposition 4.5 gives a simple connection between vectors ε and δ: $\varepsilon_i = \delta_{n-2-i}$. In other words, if $\varepsilon = (\varepsilon_1, \ldots, \varepsilon_{n-3})$, then $\delta = (\varepsilon_{n-3}, \ldots, \varepsilon_1)$. A vector δ obtained from ε in such a way we shall again denote by ε^t. Again $(\varepsilon^t)^t = \varepsilon$. Thus, a τ-code is a set $\{\varepsilon, \varepsilon^t\}$, where a vector ε is built by the rules mentioned above.

Theorem 4.7. *Two triangulanes $\boldsymbol{T} = \{T_1, \ldots, T_n\}$ and $\boldsymbol{S} = \{S_1, \ldots, S_n\}$ are r-congruent if and only if they have the same τ-code.*

Proof. Suppose first that $\boldsymbol{T}$ and $\boldsymbol{S}$ are r-congruent. Let $L(x) = P(x) + b$ be the corresponding mapping moving $\boldsymbol{T}$ onto $\boldsymbol{S}$, where P is a rotation. Without loss of generality we may assume that $L(T_1) = S_1$. That implies $L(T_i) = S_i$, and, in particular, $L(r_i) = q_i$, where r_i and q_i are the centres of triangles T_i and S_i, respectively. Since P is a rotation both the triples $r_{i+1} - r_i, r_{i+2} - r_{i+1}, r_{i+3} - r_{i+2}$ and $L(r_{i+1}) - L(r_i), L(r_{i+2}) - L(r_{i+1}), L(r_{i+3}) - L(r_{i+2})$ have the same orientation. Taking into account the equality $L(r_i) = q_i$ we get

$$g(T_i, T_{i+1}, T_{i+2}, T_{i+3}) = g(S_i, S_{i+1}, S_{i+2}, S_{i+3}).$$

Suppose now that $\boldsymbol{T}$ and $\boldsymbol{S}$ have the same τ-code. As above we may assume that

$$g(T_i, T_{i+1}, T_{i+2}, T_{i+3}) = g(S_i, S_{i+1}, S_{i+2}, S_{i+3}), \quad i = 1, \dots, n-3,$$

because a case

$$g(T_i, T_{i+1}, T_{i+2}, T_{i+3}) = g(S_{n+1-i}, S_{n-i}, S_{n-i-1}, S_{n-i-2})$$

is reduced to the last one by a renumbering $i \to n+1-i$ of triangles $S_1, \dots, S_n$.

It follows from Proposition 4.6 and Theorem 4.3 that $\boldsymbol{S}$ and $\boldsymbol{T}$ are congruent, i.e. there exist an orthogonal operator P and a vector b such that a transformation $L(x) = P(x)+b$ moves T_i onto S_i. Our proof will be completed if we shall show that P is a rotation. Consider vectors r_1, r_2, r_3, r_4 and $q_i = L(r_i)$. Since $g(T_1, T_2, T_3, T_4) = g(S_1, S_2, S_3, S_4)$, then the triples $\{r_2 - r_1, r_3 - r_2, r_4 - r_3\}$ and $\{q_2 - q_1 = L(r_2 - r_1),\ q_3 - q_2 = L(r_3 - r_2),\ q_4 - q_3 = L(r_4 - r_3)\}$ have the same orientation, whence it follows (see Proposition 4.4) that P is a rotation. □

4.3. Regular chain triangulanes

As we have seen in Section 4.1 all congruence classes of chain triangulanes with n nodes are described by means of $(n-4)$-dimensional coarse codes. What codes actually correspond to regular chain triangulanes? We still do not know the answer to this question.

Let $\boldsymbol{T} = \{T_1, \dots, T_n\}$ be a non-regular chain triangulane. That means one can find two intersecting triangles T_i, T_j with $|i-j| > 1$. It is clear that there exists at least one such a pair with minimal value of $|i-j| > 1$. Let us consider this pair of triangles. We may assume that $j > i$. By the assumption both the triangulanes $\{T_i, \dots, T_{j-1}\}$ and $\{T_{i+1}, \dots, T_j\}$ are regular. So we can say that $\{T_i, \dots, T_j\}$ is a *minimal non-regular chain triangulane* . Let us give an exact definition. A *minimal non-regular chain triangulane* (briefly *MNRC-triangulane*) $\{T_1, \dots, T_n\}$ is one which satisfies the conditions:

(i) Triangulanes $\{T_1, \dots, T_{n-1}\}$ and $\{T_2, \dots, T_n\}$ are regular;
(ii) T_1 and T_n have non-empty intersection.

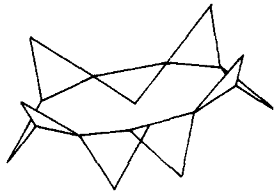

Fig. 4.

As we just have seen, any non-regular chain triangulanes contains an MNRC-triangulane. So we have the following statement.

Proposition 4.8. *A triangulane $\{T_1,\dots,T_n\}$ is regular if and only if it does not contain any MNRC-triangulane.*

We know that any chain triangulane with n triangles is uniquely determined (up to the congruence) by its coarse code which is nothing but an unordered pair of $(n-4)$-dimensional "$\pm$"-vectors $\{\chi,\chi^{\mathrm{t}}\}$ (see Section 4.1). It is easily seen from the code construction that a chain triangulane with code $\{\chi,\chi^{\mathrm{t}}\}$ contains another one with code $\{\delta,\delta^{\mathrm{t}}\}$ if and only if δ is a subsequence either of χ or of χ^{t}. Thus, to find a description of all regular chain triangulanes it is sufficient to find codes of all MNRC-ones.

The computer search arranged by one of the authors shows that the smallest example of MNRC-triangulane has 9 triangles (see Fig. 4). Its code (in terms of Theorem 4.3) is $(+,+,+,+,+)$. We conclude the paper by the following problem.

Problem. To find codes of all MNRC-triangulanes.

5. Discussion

The subject of an ideal triangulane can be further considered from different points of view. At first let us briefly discuss purely mathematical point of view. On one hand these interesting geometrical objects and their properties require to be investigated independently of possible chemical applications.

On the other hand, the triangulanes form a class of rather complicated geometrical figures built from a simple one via suitable replication. So one can generalize the notion of triangulane in the following manner. Let F be a 3-dimensional solid and $L_1,\dots,L_k$ be a finite number of affine orthogonal transformations in Euclidean space $\mathbf{R}^3$, Let $\mathcal{T}=(V,E)$ be a rooted tree whose edges $e\in E$ are labelled by transformations $L_e\in\{L_1,\dots,L_k\}$. Then one can associate with such a tree a 3-dimensional configuration of solids $F_v=L_{e_1}L_{e_2}\dots L_{e_d}(F), v\in V$, where $e_1,e_2,\dots,e_d$ is a unique way from the root of the tree to the vertex v. Now the same questions as for triangulanes may be considered.

However, all such problems are of more theoretical than practical value.

The chemical point of view is that the notion of an ideal triangulane was elaborated starting from an initial chemical experience based on small triangulanes. It was clear from the beginning that in real chemical triangulanes the actual values of lengthes of triangle side (as well as of bond and dihedral angles), can differ considerably from "standard" ones (see, e.g., data in [11]). Also every triangle has its "volume", so that the adding of hydrogene atoms can create steric obstacles and by this means influence on the existence of a particular stereoisomer. That is why the notion of an ideal triangulane was initially interpreted as a canonical representative of the class of equivalent conformations which correspond to a given stereoisomer. (Instead of the use of coarse codes which were introduced in Section 4.1 the corresponding equivalency relation can be formulated in terms of *cis/trans* disposition of triangles).

It turned out that for the case of small values of n the ideal model describes quite adequately essential features of a chemical compound from the standpoint of metrical geometry. However the existence of larger chemical triangulanes which are more strained objects (in terms of molecular mechanics) does not contradict to chemical intuition. For example, the third of authors (chemist!) conjectures that there exist chemical triangulanes whose characteristic graph includes cycles (may be of size about 10–12). Moreover, at present much work is underway to synthesize such compounds. If so, then (according to Theorem 2.1) the concept of ideal triangulane may be transformed to another one which is more flexible from the point of view of metrical geometry. However, this new generalized concept must be elaborated in such a way which for a given characteristic graph permits only a finite number of non-equivalent triangulanes.

We believe that the last problem is the most intriguing question in discussed area. One of possible ways to its solution can be based on the use of the language of abstract configurations as it is developed in [4, 8] (alternative terminology of oriented matroids can be found, e.g., in [1–3]).

In terms of abstract configurations a certain equivalence relation is established on the m-element ordered sets of points of Euclidean space. For every $m \in N$ this relation has a finite number of classes.

Let now T be a triangulane with n triangles. It is evidently completely defined by the set of vertices of triangles. Let Γ be the corresponding characteristic graph. We shall say that T is a *k-regular triangulane* if for every simple chain of length k in Γ the $(2k+1)$-element set of vertices in the corresponding chain of k triangles in T is equivalent to the set of vertices of a regular chain triangulane with k triangles. Evidently every regular triangulane which consists of n triangles is n-regular.

We believe that for sufficiently large values of k (say $k \geqslant 6$) the notion of k-regular triangulane can serve as a good initial approximation for the suitable generalizations of ideal triangulanes. Perhaps such generalization will be elaborated via dialogue between chemists and mathematicians in course of which lucky mathematical prediction will be examined in chemical laboratory.

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